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DISCLAIMER

Appendix E - First-order mass transfer coefficient estimation assuming pure diffusion

Consider purely diffusive mass transfer to the immobile region from a surrounding, constant concentration, mobile region. This one-dimensional, transient, mass diffusion problem can be stated as

$$\begin{aligned} &\frac{\partial^2 C}{\partial x^2} = \frac{1}{D^*}\frac{\partial C}{\partial t} \\ &C(0,t) = C(L,t) = C_\infty \\ &C(x,0) = C_i \end{aligned} \tag{1}$$

The problem can be made non-dimensional by defining

$$\begin{aligned} &\xi = x / L \\ &\tau = D^* t / L^2 \\ &u = \frac{C - C_\infty}{C_i - C_\infty} \end{aligned} \tag{2}$$

and equations (1) become

$$\begin{aligned} &u_{xx} = u_\tau \\ &u(0,t) = 0 \\ &u(x,0) = 1 \end{aligned} \tag{3}$$

By analogy to plane-wall transient heat conduction (Myers, 1971, section 3.1.1), the analytical solution is (Myers, 1971, equation (3.1.7))

$$u(\xi,\tau) = 4\sum_{m=0}^{\infty} \frac{\sin \beta_m \xi}{\beta_m} e^{-\beta_m^2 \tau} \tag{4}$$

where

$$\beta_m = (2m+1)\pi \tag{5}$$

The dimensional concentration becomes

$$C = C_\infty + u(C_i - C_\infty) \tag{6}$$

Under the current nomenclature, the dual-media mass transfer coefficient would be defined by

$$\theta_{im}\frac{\partial\overline{C}}{\partial t} = \beta(C_\infty - \overline{C}) \tag{7}$$

where

$$\overline{C} = \frac{\int_0^L C\theta_{im}dx}{\theta_{im}L} = \frac{1}{L}\int_0^L Cdx \tag{8}$$

Substituting (6) produces

$$\begin{aligned}\overline{C} &= \frac{1}{L}\int_0^L Cdx \\ &= \frac{1}{L}\int_0^L \left[C_\infty + u(C_i - C_\infty)\right]dx \\ &= C_\infty + (C_i - C_\infty)\frac{1}{L}\int_0^L udx \\ &= C_\infty + (C_i - C_\infty)\int_0^L ud(x/L) \\ &= C_\infty + (C_i - C_\infty)\int_0^1 ud\xi\end{aligned} \tag{9}$$

or in non-dimensional form

$$\frac{\overline{C} - C_\infty}{C_i - C_\infty} = \overline{u} = \int_0^1 ud\xi \tag{10}$$

From equation (4) the integral is evaluated as

$$
\begin{aligned}
\bar{u} &= \int_0^1 4 \sum_{m=0}^{\infty} \frac{\sin \beta_m \xi}{\beta_m} e^{-\beta_m^2 \tau} d\xi \\
&= 4 \sum_{m=0}^{\infty} \frac{1}{\beta_m} e^{-\beta_m^2 \tau} \cdot \int_0^1 \sin \beta_m \xi d\xi \\
&= 4 \sum_{m=0}^{\infty} \frac{1}{\beta_m} e^{-\beta_m^2 \tau} \cdot \left[\frac{-\cos \beta_m \xi}{\beta_m} \right]_0^1 \\
&= 4 \sum_{m=0}^{\infty} \frac{1}{\beta_m} e^{-\beta_m^2 \tau} \cdot \frac{1}{\beta_m} \left[-\cos \beta_m + 1 \right] \\
&= 4 \sum_{m=0}^{\infty} \frac{1}{\beta_m} e^{-\beta_m^2 \tau} \cdot \frac{1}{\beta_m} \left[1 + 1 \right] \\
&= 8 \sum_{m=0}^{\infty} \frac{1}{\beta_m{}^2} e^{-\beta_m^2 \tau}
\end{aligned}
\tag{11}
$$

Equation (7) can be written in a non-dimensional form as

$$
\begin{aligned}
\theta_{im} \frac{\partial \bar{C}}{\partial t} &= \beta (C_\infty - \bar{C}) \\
\frac{\partial \bar{C}}{\partial t} &= -\frac{\beta}{\theta_{im}} (\bar{C} - C_\infty) \\
\frac{\partial (\bar{C} - C_\infty)}{\partial t} &= -\frac{\beta}{\theta_{im}} (\bar{C} - C_\infty) \\
\frac{\partial (\bar{C} - C_\infty)/(C_i - C_\infty)}{\partial t} &= -\frac{\beta}{\theta_{im}} (\bar{C} - C_\infty)/(C_i - C_\infty) \\
\frac{\partial \bar{u}}{\partial t} &= -\frac{\beta}{\theta_{im}} \bar{u} \\
\frac{\partial \bar{u}}{\partial (\tau L^2 / D^*)} &= -\frac{\beta}{\theta_{im}} \bar{u} \\
\frac{\partial \bar{u}}{\partial \tau} &= -\frac{\beta L^2}{\theta_{im} D^*} \bar{u}
\end{aligned}
\tag{12}
$$

Solving for the mass transfer coefficient yields

$$
\beta = \frac{\theta_{im} D^*}{L^2 \bar{u}} \left(-\frac{\partial \bar{u}}{\partial \tau} \right) \tag{13}
$$

The time derivative is computed as

$$
\begin{aligned}
\frac{\partial \bar{u}}{\partial \tau} &= \frac{\partial}{\partial \tau}\left[8 \sum_{m=0}^{\infty} \frac{1}{\beta_m{}^2} e^{-\beta_m^2 \tau} \right] \\
&= 8 \sum_{m=0}^{\infty} \frac{1}{\beta_m{}^2} \cdot \frac{\partial}{\partial \tau} e^{-\beta_m^2 \tau} \\
&= 8 \sum_{m=0}^{\infty} \frac{1}{\beta_m{}^2} \cdot \left(-\beta_m^2 e^{-\beta_m^2 \tau} \right) \\
&= -8 \sum_{m=0}^{\infty} e^{-\beta_m^2 \tau}
\end{aligned}
\tag{11}
$$

or

$$
-\frac{\partial \bar{u}}{\partial \tau} = 8 \sum_{m=0}^{\infty} e^{-\beta_m^2 \tau} \tag{12}
$$

The dual-media mass transfer coefficient becomes

$$
\begin{aligned}
\beta &= \frac{\theta_{im} D^*}{L^2} \cdot \frac{-\dfrac{\partial \bar{u}}{\partial \tau}}{\bar{u}} \\
&= \frac{\theta_{im} D^*}{L^2} \cdot \frac{8 \displaystyle\sum_{m=0}^{\infty} e^{-\beta_m^2 \tau}}{8 \displaystyle\sum_{m=0}^{\infty} \frac{1}{\beta_m{}^2} e^{-\beta_m^2 \tau}} \\
&= \frac{\theta_{im} D^*}{L^2} \cdot \frac{\displaystyle\sum_{m=0}^{\infty} e^{-\beta_m^2 \tau}}{\displaystyle\sum_{m=0}^{\infty} \frac{1}{\beta_m{}^2} e^{-\beta_m^2 \tau}}
\end{aligned}
\tag{13}
$$

References

Myers, G. E., 1971, Analytical methods of conduction heat transfer, McGraw-Hill, New York.